Different versions that were used

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Here are some of the versions of different software that we used. More detailed description can be found in few other text files in the repository.

1 Conda/2022-09-08 on Polaris

This module was used in PointNet-Atlas and FFN Runs on Polaris. The versions of Tensorflow and PyTorch are below:

1.1 TensorFlow

- 1. tensorflow 2.10.0
- 2. tensorflow-addons 0.17.1
- 3. tensorflow-datasets 4.6.0
- 4. tensorflow-estimator 2.10.0
- 5. tensorflow-io-gcs-filesystem 0.27.0
- 6. tensorflow-metadata 1.10.0
- 7. tensorflow-probability 0.17.0

1.2 PyTorch

- $1. \ \, {\rm torch} \,\, 1.12.0 \\ {\rm a}0 + {\rm git}664058 \\ {\rm f}$
- 2. torch-geometric 2.1.0.post1
- 3. torch-scatter 2.0.9
- $4. \ \, torch\text{-sparse} \,\, 0.6.15$
- 5. torch-tb-profiler 0.4.0
- 6. torchinfo 1.7.0
- 7. torchmetrics 0.9.3

- 8. torchvision 0.13.0a0+da3794e
- 9. torchviz 0.0.2

1.3 Auxiliary

- 1. cupy-cuda116 10.6.0
- 2. h5py 3.7.0
- 3. horovod 0.25.0
- 4. hydra-colorlog 1.2.0
- 5. hydra-core 1.2.0
- 6. jax 0.3.17
- 7. jaxlib 0.3.15+cuda11.cudnn82
- 8. keras 2.10.0
- 9. keras-applications 1.0.8
- 10. keras-preprocessing 1.1.2
- 11. mpi4jax 0.3.10.post1
- 12. mpi4py 3.1.3

2 JLSE Nodes for AMD MI250

It is a little not so straightforward to run on MI250 on JLSE nodes. I had to install things on a separate environment /home/hossainm/miniconda3/envs/dist-ct-tf-amd-aux-2. Here are the versions:

2.1 TensorFlow

- 1. tensorflow-estimator 2.12.0
- 2. tensorflow-io-gcs-filesystem 0.32.0
- 3. tensorflow-rocm 2.12.0.560

and these were used with another pre-built module $\mathrm{rocm}/5.5.0$ and $\mathrm{openmpi}/4.1.1$ -llvm compiler.

2.2 PyTorch

PyTorch worked out of the box with one of the pre-built modules. That was conda/amd/2022-01-11.

- 1. torch 1.13.0+rocm5.2
- 2. torchaudio 0.13.0+rocm5.2
- 3. torchvision 0.14.0+rocm5.2

But, these were used with another pre-built module rocm/5.5.0 and openmpi/4.1.1-llvm compiler.

3 Frameworks/2023.05.15.001 on Sunspot

We used this framework module on Sunspot. The versions here are:

3.1 TensorFlow

- 1. tensorflow 2.12.0
- 2. tensorflow-estimator 2.12.0
- 3. tensorflow-io-gcs-filesystem 0.32.0

3.2 PyTorch

- 1. torch 1.13.0a0 + git6c9b55e
- 2. torchvision 0.14.1a0 + 5e8e2f1